Controlling One-Dimensional Langevin Dynamics on the Lattice

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Stochastic evolutions of classical field theories have recently become popular in the study of problems such as determination of the rates of topological transitions and the statistical mechanics of nonlinear coherent structures. To obtain high precision results from numerical calculations, a careful accounting of spacetime discreteness effects is essential, as well as the development of schemes to systematically improve convergence to the continuum. With a kink-bearing ϕ^4 field theory as the application arena, we present such an analysis for a 1+1-dimensional Langevin system. Analytical predictions and results from high resolution numerical solutions are found to be in excellent agreement.

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I. INTRODUCTION

In recent years there has been growing interest in extracting non-perturbative quantum dynamical information such as topological transition rates from numerical Langevin and Monte Carlo solutions of classical field theories at finite temperature [1]. At the next level of sophistication, several attempts have been made at developing schemes that treat low-lying modes classically and high frequency modes quantum mechanically [2]. Moreover, the equilibrium and nonequilibrium classical statistical mechanics of nonlinear coherent structures such as kinks has historically received much attention [3] in the condensed matter literature. Until fairly recently, computer memory and performance restrictions were sufficiently severe that Langevin evolutions could only be carried out at fairly low levels of accuracy and resolution. However, present-day supercomputers have overcome this problem, at least for low dimensional problems, and one can well contemplate systematically studying, understanding, and improving the accuracy of stochastic evolutions. In this paper we present just such a study applied to 1+1-dimensional Langevin systems.

Our focus will be on lattice errors for quantities computed at thermal equilibrium. In calculations of this type, a stochastic partial differential equation (SPDE) augmented with a fluctuation-dissipation relation is solved as an initial value problem using finite differences. Because of the fluctuation-dissipation relation, the system is eventually driven to thermal equilibrium and at late times one may measure values of thermodynamic quantities as well as time and space dependent correlation functions. These quantities can depend on the lattice spacing, Δx, on the total system size, on the discretization used for spatial operators, and on the timestepping algorithm used to solve the resulting set of coupled stochastic ordinary differential equations. In one space dimension a fairly complete description can be given since the question of lattice effects is one of convergence properties of SPDEs rather than of renormalization.

The configurational part of the partition function of a classical field theory in one space dimension is free from divergences. In particular, quantities such as kink densities, measured from finite difference solutions of the corresponding SPDEs, converge to a well-defined limit as the lattice spacing is reduced towards zero. The question of exactly how the convergence scales with Δx is still a matter of practical importance: numerical solutions are limited by the available computing power and memory to a finite range of values of Δx. While finite volume effects can be important in small lattices they are not important if the lattice size is much larger than the longest correlation length. We will assume that this is always the case in the considerations below.

A complete constructive procedure for determining the spatial lattice error, and possibly eliminating it to some order in Δx, exists. The method proceeds as follows. In equilibrium, the probability of a given set of configurations can be calculated from the static solution of the Fokker-Planck equation corresponding to the particular spatial discretization and time-stepping algorithm applied to the SPDE of interest. With time-stepping errors tuned to be sub-dominant, the transfer integral [4] corresponding to the lattice Hamiltonian can be evaluated to some given order in Δx. Correlation functions and thermodynamic quantities, which can all be extracted from the transfer integral, explicitly exhibit lattice dependences allowing the convergence to the continuum to be read off directly. We describe this procedure in more detail below.

Discreteness effects have been considered before in the context of kink dynamics [5]. Trullinger and Sasaki have already obtained the lowest-order discreteness corrections to the Schrödinger equation that emerges from the transfer integral approach [6]. They found that the lowest order correction is of order Δx^2 and, in first-order

perturbation theory, is equivalent to a corrected effective potential. As we show below, the latter result can be adapted not only to compute the order of the lattice errors but also to introduce a local counterterm in the stochastic evolution equations that can drastically improve the convergence to the continuum. Our results from high resolution numerical solutions are in excellent agreement with the theoretical predictions.

The class of problems considered here are 1+1-dimensional classical field theories defined by the Hamiltonian:

$$H = \int \mathrm{d}x \left[\frac{1}{2}\pi^2 + \frac{1}{2}\left(\frac{\partial \Phi}{\partial x}\right)^2 + V(\Phi) \right] . \tag{1}$$

The corresponding continuum SPDE

$$\frac{\partial^2}{\partial t^2}\Phi(x) = \frac{\partial^2}{\partial x^2}\Phi(x) - \eta\frac{\partial}{\partial t}\Phi(x) - \frac{\delta}{\delta\Phi}V(\Phi) + F(x,t) \tag{2}$$

is second order in time, where with $\beta = 1/kT$, the noise and damping obey a fluctuation-dissipation relation:

$$\langle F(x,t)F(y,s)\rangle = 2\eta\beta^{-1}\delta(t-s)\delta(x-y) \ . \tag{3}$$

In this paper we will adopt the example of the double-well Φ^4 theory: $V(\Phi) = -(m^2/2)\Phi^2 + (g^2/4)\Phi^4$. We shall work in a dimensionless form of the theory given by the transformations: $\phi = \Phi/a$, $\bar{x} = mx$, and $\bar{t} = mt$, where $a^2 = m^2/g^2$. Under these transformations, the original Hamiltonian becomes $\bar{H} = H/(ma^2)$ where $\bar{H}$ is of the same form as the original Hamiltonian H, except that the potential $V(\phi) = -(1/2)\phi^2 + (1/4)\phi^4$.

This theory admits the well-known (anti-)kink solutions which, at zero temperature, are exact solutions of the static field equations connecting $\phi = -1$ at $x = (+) - \infty$ to $\phi = +1$ at $x = (-) + \infty$. In thermal equilibrium, the balance between noise and damping is manifested in the balance of nucleation and annihilation of kink-antikink pairs [7]. At low temperature, WKB techniques applied to the transfer integral [8,9] yield the following approximation for the density of kinks:

$$\rho_k \propto (E_k/kT)^{1/2}\exp(-E_k/kT), \tag{4}$$

where $E_k = \sqrt{8/9}$, the energy of an isolated kink. Supporting numerical evidence exists [10], but precise results have been difficult to obtain until recently due to the large amount of computing time needed at temperatures low enough to clearly distinguish kinks. The best results obtained so far are for a special double-well potential where exact theoretical computations can also be carried out. In this case, it has been shown that the theoretical and numerical results agree within statistical bounds set by the finite volume of the simulations [11].

The classical partition function for a ϕ^4 theory, in any spatial dimension $2 \leq D < 4$, is super-renormalizable, i.e., there are a finite number of perturbative diagrams that are divergent in the continuum, but can be appropriately subtracted by the inclusion in the theory of a finite number of suitable counterterms. The situation is different for $D = 1$: the continuum partition function is finite and no renormalization is necessary.

An alternative approach to the one described here has been suggested by Gleiser and Müller [12] who have proposed a perturbative counterterm for use in 1+1-dimensional Langevin equations. A weakness of the latter proposal is that it relies on an approximation to the free energy; in many situations the latter is a poor indicator of the true dynamics of field theories [13]. Moreover, their counterterm is based on an approximate effective potential calculated by perturbing about a uniform state. We will show below, with both analytic and numerical results, the inadequacy of perturbative counterterms in dealing with the convergence to the continuum.

The paper is organized as follows. In Section II we consider the evolution of the probability density of the discretized SPDE. We use the method of Horowitz [14] to examine the effect of time discretization on the equilibrium density. The transfer integral is introduced in Section III. We perform calculations at finite Δx and show that the leading order corrections to the continuum of observable quantities are proportional to Δx^2. Examination of the form of the Schrödinger equation at finite Δx reveals a natural choice for a local counterterm with which to improve the convergence properties of discretized Langevin equations. The alternative one loop approach of Gleiser and Müller is examined in Section IV. Numerical results are presented in Section V. In Section VI we end with a discussion of our results.

II. THE DISCRETE TIME FOKKER-PLANCK EQUATION

Our first step in determining the (equilibrium canonical) distribution to which a given Langevin dynamics converges for long times is to derive the corresponding Fokker-Planck equation. This can be done on the lattice as well as in the continuum.

On the lattice, an SPDE is solved by updating $2N$ quantities $\{\phi_i(t), \pi_i(t)\}$ where $i = 1, \ldots, N$. We take the lattice Hamiltonian in one space dimension, H_{lat}, to be

$$H_{\mathrm{lat}} = \Delta x \sum_{i=0}^{N} \left[\frac{1}{2}\pi_i^2 + S(\phi_i) \right], \tag{5}$$

with

$$S(\phi_i) = \frac{1}{2}\frac{(\phi_{i+1} - \phi_i)^2}{\Delta x^2} + V(\phi_i), \tag{6}$$

$$V(\phi_i) = -\frac{1}{2}\phi_i^2 + \frac{1}{4}\phi_i^4. \tag{7}$$

The corresponding Fokker-Planck equation for the $2N$ variables has a static solution that can in principle be

attained at late times in a Langevin simulation (in the sense of ensemble averages over individual simulations).

In practice the time as well as the space discretization of a Langevin equation leads to errors. The simplest stochastic timestepping is of the Euler type and can be written as:

$$\pi_i(t+\Delta t) = \pi_i(t) - \Delta t\left[\eta\pi_i(t) - \frac{\partial H_{\rm lat}}{\partial\phi_i(t)}\right] + \xi_i(t),$$
$$\phi_i(t+\Delta t) = \phi_i(t) + \Delta t\pi_i(t). \tag{8}$$

We have chosen the case of additive Gaussian white noise, related to the damping η by the (suitably discretized) fluctuation-dissipation relation:

$$\langle\xi_t(t)\rangle = 0, \quad \langle\xi_i(t)\xi_j(t')\rangle = \frac{2\eta}{\beta}\frac{1}{\Delta t\Delta x}\delta_{ij}\delta_{tt'}. \tag{9}$$

In order to understand the effect of time discretization, it is possible write a discrete time Fokker-Planck equation, describing the evolution of the probability density functional associated with (8)-(9) [14]:

$$P[\{\pi,\phi\},t+\Delta t] = \exp\left(-\Delta t\frac{\partial}{\partial\phi_i}\frac{\partial H_{\rm lat}}{\partial\pi_i}\right)\times \tag{10}$$
$$\exp\left[\Delta t\frac{\partial}{\partial\pi_i}\left(\eta\frac{\partial H_{\rm lat}}{\partial\pi_i}+\frac{\partial H_{\rm lat}}{\partial\phi_i}\right)+\Delta t\frac{\eta}{\beta}\frac{\partial^2}{\partial\pi_i^2}\right]P[\{\pi,\phi\},t],$$

where summation over repeated indices is implied. For simplicity this will be assumed in what follows and indices dropped. The discrete time equation (10) can be written in the form

$$P[\{\pi,\phi\},t+\Delta t] = e^{-\Delta t H_{\rm FP}}P[\{\pi,\phi\},t]. \tag{11}$$

The operators in the two exponents in (10) are non-commuting. To reduce (10) to the form (11) we use the Campbell-Baker-Hausdorff theorem: given the operators A and B, there is (formally) an operator C such that $e^Ae^B = e^C$, with

$$C = \quad A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]]$$
$$+\frac{1}{12}[B,[B,A]] + \dots \tag{12}$$

Expanding to first order in Δt, we have

$$H_{\rm FP} = \frac{\eta}{\beta}\frac{\partial^2}{\partial\pi^2} - \frac{\partial H_{\rm lat}}{\partial\pi}\frac{\partial}{\partial\phi} + \frac{\partial}{\partial\pi}\left(\eta\frac{\partial H_{\rm lat}}{\partial\pi}+\frac{\partial H_{\rm lat}}{\partial\phi}\right)$$
$$+\frac{1}{2}\Delta t\left[\eta\frac{\partial H_{\rm lat}}{\partial\pi}+\frac{\eta}{\beta}\frac{\partial}{\partial\pi}+\frac{\partial H_{\rm lat}}{\partial\phi}\right]\frac{\partial}{\partial\phi} \tag{13}$$
$$-\frac{1}{2}\Delta t\ \frac{\partial H_{\rm lat}}{\partial\pi}\frac{\partial^2 H_{\rm lat}}{\partial\phi^2}\frac{\partial}{\partial\pi} + \mathcal{O}(\Delta t^2).$$

Notice that each factor of $H_{\rm lat}$ introduces a power of Δx.

The solution of $H_{\rm FP}P[\{\phi,\pi\}] = 0$ is the canonical distribution approached by the discretized system at late times. Its form can be computed for small Δt. To zeroth order for the momenta and order Δt for the fields we obtain

$$P[\{\pi,\phi\}] = \exp\Big(-\Delta x\sum_i\big[\beta'\frac{\pi_i^2}{2}+\beta S(\phi_i) \tag{14}$$
$$-\Delta t\frac{\beta}{2}\pi_i\frac{\partial S}{\partial\phi_i}\big]\Big),$$

where $\beta' = \beta\left(1+\Delta t\frac{\eta}{2}\right)$. Note that the discretization induces cross terms between ϕ and π in the canonical distribution. This is a general feature of higher order solutions in Δt. (These terms rapidly become very complicated.) Different time discretizations lead to different discrete time Fokker-Planck equations. The numerical simulations described below employed a stochastic second order Runge-Kutta algorithm [15].

The equilibrium density of configurations of the space- and time-discretized theory, is obtained by performing the Gaussian integral over the momenta in (14):

$$P[\{\phi\}] = A\exp\left[-\beta\Delta x\sum_i\left\{S(\phi_i)-\frac{\Delta t^2}{8}\left(\frac{\partial S}{\partial\phi_i}\right)^2\right\}\right]. \tag{15}$$

The effect of the time discretization is explicitly seen as a modification of the equilibrium density. Further integration of (14) cannot be performed so easily because each $S(\phi_i)$ depends also on ϕ_{i+1}.

The functional integral of $P[\phi]$ over ϕ defines the configurational partition function

$$Z_\phi = Z_\pi\int D\phi e^{-\beta S[\phi]} = \prod_{i=1}^N\int d\bar{\phi}_i e^{-\beta\Delta S[\phi_{i+1},\phi_i]}. \tag{16}$$

which we study in the next section. Here $d\bar{\phi}_i = \bar{N}d\phi_i$, with $\bar{N} = \sqrt{\frac{\beta}{2\pi\Delta x}}$.

In principle, the partition function as calculated above would include artifacts from both the time and space discretizations. In actual computational practice, given that we can estimate the order of the time stepping errors as shown already, it is not difficult to reduce the time step to a level where the remaining errors are suppressed compared to the errors from the spatial discretization. Once this is done, we may safely ignore the discretization in time and concentrate solely on the errors due to the spatial lattice.

III. THE TRANSFER INTEGRAL

To compute the partition function explicitly we make use of the transfer integral method [4]. The configurational partition function Z_ϕ is given by

$$Z_\phi = \int_{-\infty}^{\infty}d\bar{\phi}_1\dots d\bar{\phi}_N\prod_{i=1}^N T(\phi_i,\phi_{i+1}), \tag{17}$$

where

$$T(\phi_i,\phi_{i+1}) = \exp\left\{-\frac{1}{2}\beta\Delta x\left[\left(\frac{\phi_{i+1}-\phi_i}{\Delta x}\right)^2 + V(\phi_i)+V(\phi_{i+1})\right]\right\}$$

and $\phi_{N+1}=\phi_1$ implements spatially periodic boundary conditions. The difficulty with evaluating Z_ϕ lies in the coupling of integrals at different space points. The idea behind the transfer operator method is to "localize" the evaluation of the integrals in (17).

The transfer operator $\hat{T}$ is defined as follows

$$\hat{T}\psi(\phi_{i+1}) = \int_{-\infty}^{\infty} \mathrm{d}\bar{\phi}_i T(\phi_i,\phi_{i+1})\psi(\phi_i). \tag{18}$$

Suppose we can find the eigenvalues of $\hat{T}$. That is, suppose we can solve the following Fredholm equation:

$$\int_{-\infty}^{\infty} \mathrm{d}\bar{\phi}_i T(\phi_i,\phi_{i+1})\psi_n(\phi_i) = t_n\psi_n(\phi_{i+1})\ , \tag{19}$$

where the t_n are positive constants that we write for later convenience as

$$t_n = \mathrm{e}^{-\beta\Delta x\epsilon_n}. \tag{20}$$

Then

$$Z_\phi = \sum_n t_n^N. \tag{21}$$

In the limit $N\to\infty$, the sum (21) is dominated by the largest eigenvalue:

$$Z_\phi = \sum_n t_n^N \to t_0^N = \mathrm{e}^{-\beta L\epsilon_0}, \tag{22}$$

where $L=N\Delta x$ is the physical length of the lattice. In the thermodynamic limit $L\to\infty$, the free energy density is simply $F_\phi=\epsilon_0$. It is clear that once the partition function is known in the thermodynamic limit we may compute from it any thermodynamic quantity. Moreover, it is possible to show that spatial, and in linear response theory, temporal correlation functions can also be computed via a knowledge of the spectrum of the transfer operator [16].

We now turn to the procedure for solution of (19) by first converting it into an infinite order partial differential equation. We first rewrite (19) as

$$\begin{aligned}&\mathrm{e}^{-\frac{1}{2}\beta\Delta x V(\phi_{i+1})}\times\\ &\int \mathrm{d}\bar{\phi}_i\ \mathrm{e}^{-\frac{\beta}{2\Delta x}(\phi_{i+1}-\phi_i)^2}\mathrm{e}^{(\phi_i-\phi_{i+1})\partial/\partial\phi_{i+1}}\chi(\phi_{i+1})\\ &= \mathrm{e}^{-\beta\Delta x\epsilon_n}\psi_n(\phi_{i+1})\ ,\end{aligned} \tag{23}$$

where

$$\chi(\phi) = \mathrm{e}^{-\frac{1}{2}\beta\Delta x V(\phi)}\psi_n(\phi). \tag{24}$$

The special form of the Fredholm kernel has led to a simple Gaussian integral that yields:

$$\begin{aligned}&\mathrm{e}^{-\frac{1}{2}\beta\Delta x V(\phi_{i+1})}\mathrm{e}^{(\Delta x/2\beta)\partial^2/\partial\phi_{i+1}^2}\left(\mathrm{e}^{-\frac{1}{2}\beta\Delta x V(\phi_{i+1})}\psi_n(\phi_{i+1})\right)\\ &= \mathrm{e}^{-\beta\Delta x\epsilon_n}\psi_n(\phi_{i+1})\ .\end{aligned} \tag{25}$$

This (exact) result yields the form $\mathrm{e}^U\mathrm{e}^D\mathrm{e}^U\psi = \mathrm{e}^C\psi$ where U and D are operators and C is a real number. The Campbell-Baker-Hausdorff series in this case is formally an expansion in powers of Δx. To linear order in Δx, the CBH expansion applied to (25) yields:

$$\mathrm{e}^{-\beta\Delta x V(\phi)+\frac{\Delta x}{2\beta}\frac{\partial^2}{\partial\phi^2}}\psi_n(\phi) = \mathrm{e}^{-\beta\Delta x\epsilon_n}\psi_n(\phi)\ , \tag{26}$$

or equivalently

$$\left[-\frac{1}{2\beta^2}\frac{\partial^2}{\partial\phi^2}+V(\phi)\right]\psi_n = \epsilon_n\psi_n\ . \tag{27}$$

The transfer integral technique thus reduces the calculation of Z_ϕ to the calculation of the eigenvalues ϵ_n of a corresponding Schrödinger equation:

$$\left\{-\frac{1}{2\beta^2}\frac{\partial^2}{\partial\phi^2}+U(\phi,\Delta x)\right\}\psi_n = \epsilon_n\psi_n\ , \tag{28}$$

where $U(\phi,0)=V(\phi)$. The calculation is explicitly performed on the lattice, at finite Δx: leading order corrections to the eigenvalues of the Schrödinger equation (28) are proportional to Δx^2. For the problem at hand, one finds [6],

$$\begin{aligned}&\left\{-\frac{1}{2\beta^2}\frac{\partial^2}{\partial\phi^2}+V(\phi)+\frac{1}{6}(\Delta x)^2\left[\frac{1}{4}\left(\frac{\partial V}{\partial\phi}\right)^2\right.\right.\\ &\left.\left.+\frac{1}{2\beta^2}\frac{\partial^2 V}{\partial\phi^2}\frac{\partial^2}{\partial\phi^2}+\frac{1}{2\beta^2}\frac{\partial^3 V}{\partial\phi^3}\frac{\partial}{\partial\phi}+\frac{1}{8\beta^2}\frac{\partial^4 V}{\partial\phi^4}\right]\right\}\psi_n = \epsilon_n\psi_n\ .\end{aligned} \tag{29}$$

Higher order corrections in Δx in (29) can be computed in a tedious though straightforward fashion by going to higher orders in the CBH expansion. It is easy to show from the symmetric form of (25) and the Hermitian/anti-Hermitian alternation of terms in the CBH expansion that the error terms are always of even order in powers of Δx. Thus, if a method is found to cancel errors up to a certain order m, it automatically reduces the error to order $m+2$.

The simplest example of Δx dependence is the free theory: $V=\frac{1}{2}\phi^2$. Then (29) reduces to

$$\left[-\frac{1}{2\beta'^2}\frac{\partial^2}{\partial\phi^2}+\frac{1}{2}m'^2\phi^2\right]\psi_n = \epsilon_n\psi_n, \tag{30}$$

with $\beta'=\beta/\sqrt{1-a}$, $m'=\sqrt{1+a/2}$ and $a=(\Delta x)^2/6$. This implies in particular for the energy spectrum $\epsilon_n = \left(n+\frac{1}{2}\right)\frac{m'}{\beta'} \simeq (n+\frac{1}{2})\frac{1}{\beta}\left(1-\frac{1}{24}(\Delta x)^2\right)$. The free theory is a convenient special case because the corresponding SPDE is linear and exactly solvable. Quantities such as

$\langle \phi^2(x) \rangle$ can be evaluated exactly and compared to the results from the transfer integral. Both procedures agree, and

$$\langle \phi^2(x) \rangle = \frac{1}{2\beta} \frac{1}{\sqrt{1+\frac{\Delta x^2}{4}}} = \frac{1}{2\beta}\left(1 - \frac{1}{8}\Delta x^2\right) + O(\Delta x^4). \tag{31}$$

Note that the leading dependence on lattice spacing is proportional to Δx^2.

We now turn to the question of lattice errors in determining the kink density, which, at sufficiently low temperatures, is controlled completely by the correlation length derived from the two-point function $\langle \phi(0)\phi(x) \rangle$. Applying the transfer integral formalism, it is easy to show that this correlation function is a sum of exponentials with exponents proportional to differences of eigenvalues of (28). The correlation length is determined by the energy difference between the ground and first excited states of (28) [4]. At low temperatures, the WKB (or semiclassical) approximation is excellent and this energy difference is the exponentially small tunnel-splitting term. Note that at low temperatures the kink density is given directly by the correlation length, $\rho_k \simeq 1/(4\lambda_\infty)$ [10].

At low temperatures the first two eigenfunctions of (27) are of the form

$$\begin{aligned} \psi_S &= \frac{1}{\sqrt{2}}(\psi_L + \psi_R), \\ \psi_A &= \frac{1}{\sqrt{2}}(\psi_L - \psi_R), \end{aligned} \tag{32}$$

where ψ_S is the (symmetric) ground state and ψ_A is the (antisymmetric) first excited state. Here ψ_L and ψ_R are the usual localized states, one on each side of the barrier. To estimate the error due to finite lattice spacing we use first order perturbation theory in $(\Delta x)^2$. The corrected energies are then,

$$\begin{aligned} E_0^{(\Delta x)} &= E_0 + \langle \psi_S | \delta H | \psi_S \rangle, \\ E_1^{(\Delta x)} &= E_1 + \langle \psi_A | \delta H | \psi_A \rangle, \end{aligned} \tag{33}$$

where E_0 and E_1 are the results from the continuum theory and $\delta H \sim O(\Delta x^2)$ is the error Hamiltonian. It follows that the energy difference is

$$\Delta E_{10}^{(\Delta x)} = \Delta E_{10} - 2\langle \psi_L | \delta H | \psi_R \rangle. \tag{34}$$

The error Hamiltonian can be read off from (29) and it is clear that the error in energy differences, and hence kink density at low temperatures, is also $O(\Delta x^2)$ at leading order. Corrections to the the eigenstates lead to higher order Δx dependences.

More generally, given any eigenvector $|\psi\rangle$ of the continuum Schrödinger equation, for the specific form of δH of (29), integration by parts and use of (28) yields [6],

$$\langle \psi | \delta H | \psi \rangle = -\frac{(\Delta x)^2}{24} \langle \psi | \left(\frac{\delta V}{\delta \phi}\right)^2 | \psi \rangle. \tag{35}$$

Apart from the eigenvectors, there is no temperature dependence in (35). This remarkable fact immediately suggests the introduction of a counterterm in the lattice equations which, in perturbation theory, would lead to the cancellation of errors of order $(\Delta x)^2$. Modifying the potential as follows

$$V(\phi) = V(\phi) - \frac{(\Delta x)^2}{24}\left(\frac{\delta V}{\delta \phi}\right)^2, \tag{36}$$

leads to the cancellation of lattice dependences to order $(\Delta x)^2$ in a way that preserves the fluctuation-dissipation relation (taken at any temperature) and is thus suited for dynamics as well as thermodynamics. With Δx taken to be small enough, the leading error now becomes dominantly $O(\Delta x)^4$. We note that unlike the situation for PDEs where one improves the lattice approximation for spatial derivatives, here a local counterterm produces the same effect.

In the specific case of a ϕ^4 potential, the counterterm (36) gives a new potential including the term $-\Delta x^2 \phi^6/24$. The corrected potential is thus unbounded from below! In first order perturbation theory this is not a problem since the corresponding wave function is exponentially small in the pathological region of the compensated potential [6]. However, if the full potential is to be used in a Langevin simulation it is clear that at sufficiently long times, the unboundedness of the potential implies the nonexistence of a stable thermal distribution. Fortunately, it is simple to estimate whether this problem actually shows up in real simulations. The answer, as we show below, is that it is of absolutely no practical significance in the parameter range of interest.

The resolution of this apparent difficulty brings us back to the validity of the expansion in Δx. So far we have implicitly assumed that $\beta \simeq 1$, so that Δx is the only small parameter and controls the order of the expansion. If on the other hand one wanted to work in a regime where $\Delta x \geq \beta$, the whole expansion in Δx would have to be rederived in terms of an appropriate small parameter. In any case this latter regime would always constitute a poor approximation to the continuum: It is the Ising (disorder) limit of the field theory.

A simple argument for why the counterterm works at small temperatures, meaning $\Delta x \ll \beta$, is the following. Consider a temperature large relative to the potential barrier between the minima. Then, from the uncorrected eigenvalue equation, $\langle \phi(x)^2 \rangle \simeq \beta^{-1}$. On the other hand the value of $\phi(x)^2$ for which a fluctuation can probe the effect of the negative ϕ^6 term at large ϕ is $\phi^2(x) \simeq 6/(\Delta x)^2$. Therefore the condition for the negative ϕ^6 term not to affect the evolution is $\Delta^2 x \ll 6\beta$. At lower temperatures it is more appropriate to explicitly calculate the Kramers escape rate [17] across the barrier separating the metastable and unstable regions of

the compensated potential. Assuming the lattice sites to be uncoupled (this gives an overestimate of the true rate), the calculation yields $\Gamma_K \sim \exp(-4\beta/3(\Delta x)^4)$, which turns out to be vanishingly small in practice: For $\Delta x = .5$, $\beta = 5$, and a lattice size of 10^6 points, the probability of an escape at a single site per unit time is only $\sim 10^{-41}$. In our numerical calculations we have verified that the counterterm can indeed be successfully used in the appropriate circumstances with no hint of any instabilities.

IV. THE ONE LOOP APPROACH

In contrast to the above considerations, the 1-loop counterterm proposed in Ref. [12] arises from the conjecture that the leading dependence of the partition function on Δx coincides with the most divergent term for the same theory in higher dimensions. Although the relevant computations are well known we will spell out some of the steps to make every assumption clear. The basic idea is to start again with the canonical partition function:

$$Z = N \int D\phi e^{-\beta S[\phi]} \ . \tag{37}$$

The field ϕ is then decomposed into a background field ϕ_b and a fluctuation field χ, $\phi = \phi_b + \chi$, and assuming the fluctuations to be small, expanded around ϕ_b:

$$S[\phi_b + \chi] \approx S[\phi_b] + \frac{\delta S}{\delta \phi}_{|\chi=0} \chi + \frac{1}{2}\chi \frac{\delta^2 S}{\delta \phi^2}_{|\chi=0} \chi + \ldots . \tag{38}$$

If ϕ_b is an extremum of $S[\phi]$ then the first term vanishes. Under this assumption

$$Z = N e^{-\beta S[\phi_b]} \int D\chi e^{-\beta \frac{1}{2}\chi \frac{\delta^2 S}{\delta \phi^2}_{|\chi=0} \chi} . \tag{39}$$

Because $\frac{\delta^2 S}{\delta \phi^2}_{|\chi=0}$ is independent of χ the functional integration is strictly Gaussian and can be performed exactly:

$$N \int D\chi e^{-\beta \frac{1}{2}\chi \frac{\delta^2 S}{\delta \phi^2}|_{\chi=0} \chi} = \mathrm{Det}^{-1/2}\left(\frac{S_I''}{S_0''}\right) . \tag{40}$$

Here we have adopted the usual normalization to the free theory. The action $S = S_0 + S_I$, was decomposed into the action for the free theory S_0 (gradient and mass terms) and the interactions S_I. Primes denote functional derivatives relative to ϕ.

This can be written as

$$\begin{aligned} \mathrm{Det}^{-1/2}\left(\frac{S''}{S_0''}\right) &= \mathrm{Det}^{-1/2}(1+K) \\ &= e^{-\frac{1}{2}\mathrm{Tr}\log(1+K)}, \end{aligned} \tag{41}$$

where $K = S_I''/S_0''$. Performing the 1D k-space trace integral, ($m = 0$), with an ultraviolet cutoff $\Lambda = \pi/\Delta x$, we obtain one loop corrections to the potential

$$V_{1L}(\phi, \Lambda) = V_0 + \frac{T}{4}\sqrt{S_I''(\phi_b)} - \frac{T\Delta x}{4\pi^2} S_I''(\phi_b) \ . \tag{42}$$

The partition function is now approximately given by

$$Z = e^{-\beta S[\phi_b] + \frac{1}{4\beta}\sqrt{S_I''(\phi_b)} - \frac{\Delta x}{4\beta\pi^2} S_I''(\phi_b)} \ . \tag{43}$$

Equations (42) and (43) constitute the basis for the proposal of Ref. [12]. In order to cancel the leading Δx dependence arising in this scheme, the original bare potential is modified by the addition of the last term in Eq. (42), (with a positive sign).

Notice that while a careful accounting of the dynamics on the lattice yields a leading correction of order $(\Delta x)^2$, regardless of any assumptions about the dominant thermodynamic field configurations, the one loop procedure leads to a correction of order Δx. In contrast to the correct answer discussed in the previous section, the one loop procedure gives no corrections for the free theory since in this case $S_I \equiv 0$.

V. COMPARISON WITH NUMERICAL SOLUTIONS

Accurate Langevin studies of even one-dimensional field theories require large lattices and long running times. It has only recently been realized, by comparison against exact analytic results for nonlinear field theories, that fairly large errors (e.g., 30% or greater in the kink density) can easily arise if numerical studies are not carried out with careful error control methodologies [11].

In order to test the predictions of the previous sections, we ran large scale Langevin evolutions with typical lattice sizes $N = 10^6$, and with the time step related to the lattice spacing by $\Delta t = 0.05\Delta x^2$.

A first test which allows comparison against exact analytical results are the lattice dependences for the linear SPDE (free theory) defined by $V(\phi) = \phi^2/2$. Figure 1 shows the plot of the thermal equilibrium $1 - \langle \phi^2 \rangle$ versus Δx. The numerical data are in excellent agreement with the (exact) theoretical predictions.

In the more general case of a nonlinear SPDE, we cannot expect explicit exact solutions for arbitrary Δx, but thermodynamic quantities can be obtained to order Δx^2 from the eigenvalues of the perturbed Schrödinger equation extracted from the transfer integral, as described in Section III. In the case of predictions for the kink density, precise comparison with numerical results has not been possible until recently, partly due to the difficulty of counting the number of kinks in a noisy configuration. The correlation length is, however, a well-defined quantity at any temperature, independent of kink-counting schemes.

We extract the correlation length λ_∞ from the numerically determined field configurations as follows. Let

$$c(i\Delta x) = \langle \phi(j)\phi(j+i) \rangle, \tag{44}$$

and

$$\lambda(x) = \Delta x \left(\log \left(\frac{c(x)}{c(x+\Delta x)} \right) \right)^{-1}. \tag{45}$$

The correlation length is $\lim_{x\to\infty} \lambda(x)$:

$$\langle \phi(0)\phi(x) \rangle \to \exp\left(-x/\lambda_\infty\right), \qquad x \to \infty. \tag{46}$$

The correlation function $c(x)$ is in general a sum of exponentials (the smallest exponent being the correlation length). For values of x much smaller than the correlation length, therefore, $\lambda(x) < \lambda_\infty$. In practice, for large x, finite statistics mean that the ratio in (45) cannot be evaluated precisely. One therefore evaluates the correlation length by plotting $\lambda(x)$ versus x and looking for a plateau at intermediate values of x.

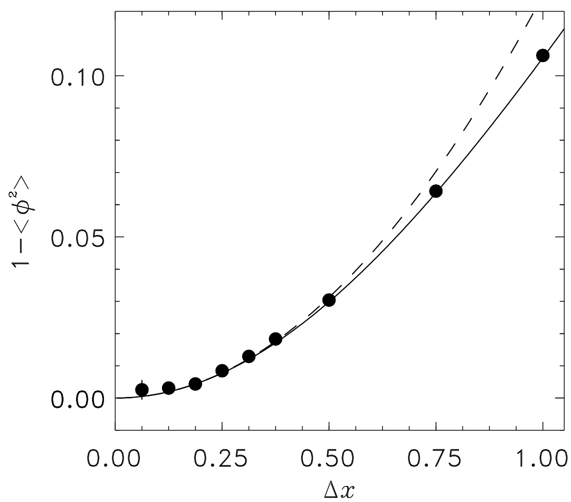

FIG. 1. The dependence of $1 - \langle \phi^2 \rangle$ on Δx, for $V(\phi) = \phi^2/2$. The numerical results ($\bullet$) at $\beta = 2$ are compared with the exact equilibrium result (31) (solid line). The dashed line shows the Taylor expansion of (31) to order Δx^2. Statistical error bars are not shown if they are smaller than the symbol size.

We measured the correlation length using three different Langevin evolutions: (a) A standard simulation using a second-order stochastic Runge-Kutta integrator; (b) A simulation with the counterterm (36); (c) A simulation with the counterterm proposed in Ref. [12]. Results for $\Delta x = 0.5$ are shown in Figure 2. The counterterm (36) shifts the result from the Langevin evolutions (a) on the lattice very close to the exact continuum result, shown as a dashed line. The standard simulation overestimates λ_∞, whereas the one loop counterterm results in an underestimate with an error larger than the "bare" simulation (a) without any counterterm.

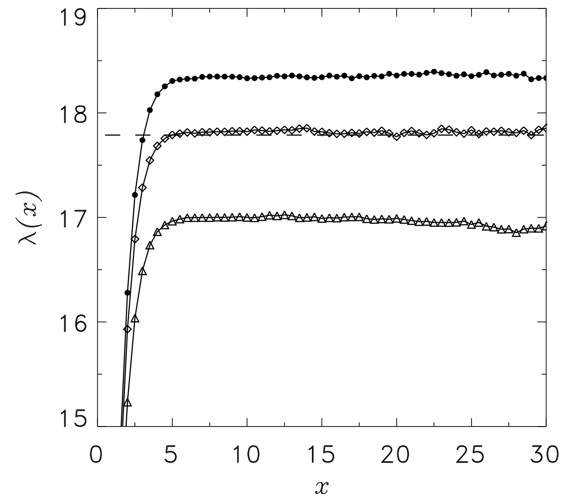

FIG. 2. The correlation length λ computed with the bare potential ($\bullet$), the counterterm of (36) ($\diamond$) and the one loop counterterm ($\triangle$), for $\Delta x = 0.5$ and $\beta = 5$. The dashed line shows the continuum exact result, computed via the transfer integral.

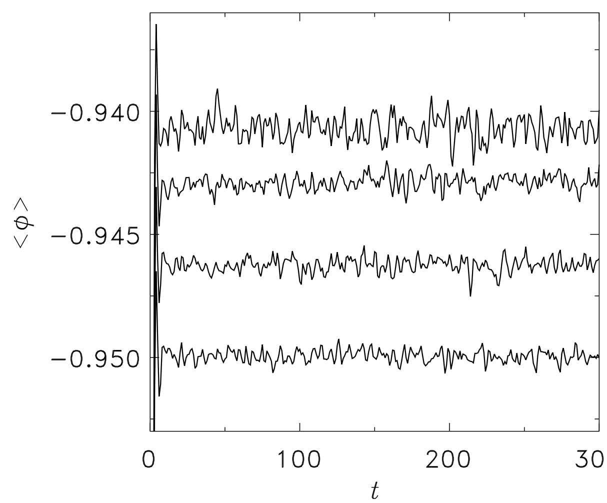

FIG. 3. Early evolution of the space-averaged mean value of ϕ for different values of the lattice spacing Δx. From top to bottom, the lattice spacings are: $\Delta x = 0.25,\ 0.5,\ 0.75,\ 1.0$. We used lattices of 1048576 points and $\Delta t = 0.05\Delta x^2$. $\beta = 10$, $\eta = 1$.

As a further test we repeated, with large lattices and smaller time steps, a numerical experiment presented in Ref. [12]. The initial condition is chosen uniform at the minimum of $V(\phi)$, $\phi_0 = -1$; the system is then run for a short time (before any kinks appear) so as to observe the relaxation to a mean value ϕ_m. Although this does not result in a strictly thermalized configuration, small wave-length fluctuations quickly display a thermal spec-

trum. (In other words, the "phonon" relaxation time is much smaller than the timescale for kink nucleation.) In Figure 3 we show the value of $\langle\phi\rangle$ as a function of time for four values of Δx. From the plateau for moderate times, we can obtain a fairly precise estimate of ϕ_m. As a cautionary note, we point out that at small Δx, a small stepsize is also needed (see Figure 4).

It is possible to employ a Gaussian approximation (following Ref. [10]) to obtain a rather good estimate of ϕ_m as a function of Δx, the result being shown in Figure 5: The leading dependence, both analytically and numerically, is clearly quadratic in Δx. To obtain the analytic result, we use the fact that the probability density of ϕ is the square of the ground state of the Schrödinger equation (28). (This density emerges from dynamic simulations or calculations; it is not an input to numerics.)

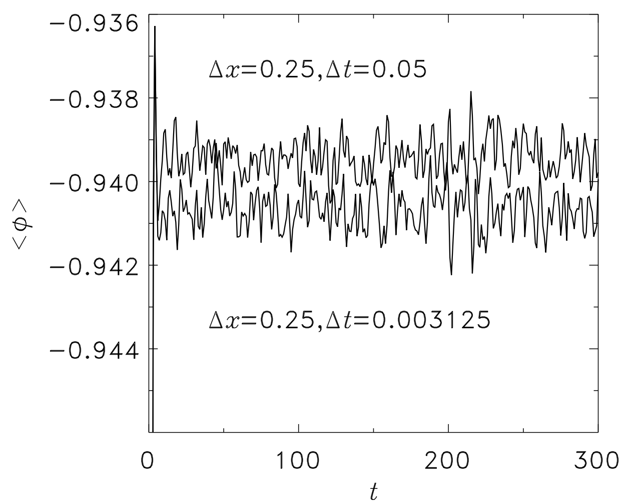

FIG. 4. Early evolution of the space-averaged mean value of ϕ for two values of the time step Δt, with $\beta = 10$, $\eta = 1$.

We proceed further by using a Gaussian ansatz [10] for the ground state eigenfunction:

$$\psi_0(\phi) = \left(\frac{\Omega}{\pi}\right)^{\frac{1}{2}} \exp(-\frac{1}{2}\Omega(\phi-\phi_0)^2). \tag{47}$$

The parameters Ω and ϕ_0 are obtained by minimizing the energy

$$E_0 = \int_{-\infty}^{\infty} \psi_0^2(\phi) H(\phi) \mathrm{d}\phi. \tag{48}$$

For large β the two free parameters are related by

$$\Omega = \beta\left(3\phi_0^2 - 1\right)^{\frac{1}{2}} + \mathcal{O}(1), \tag{49}$$

and

$$E_0 = -\frac{1}{2}\phi_0^2 + \frac{1}{4}\phi_0^4 + \beta^{-1}\frac{1}{2}(3\phi_0^2-1)^{\frac{1}{2}} + \mathcal{O}(\beta^{-2}). \tag{50}$$

The dependence of ϕ_m on Δx can now be estimated using the Gaussian approximation of (47). At finite Δx, we replace $V(\phi)$ in (48) by $V(\phi) + \frac{1}{24}\Delta x^2(\frac{\delta}{\delta\phi}V(\phi))^2$. Minimizing (50) with respect to ϕ_0 gives

$$\phi_0(\Delta x) = \phi_0(0) + \beta^{-1}\Delta x^2 \frac{11}{64\sqrt{2}} + \mathcal{O}(\beta^{-2}) , \tag{51}$$

which is plotted in Figure 5, in excellent agreement with the numerical results.

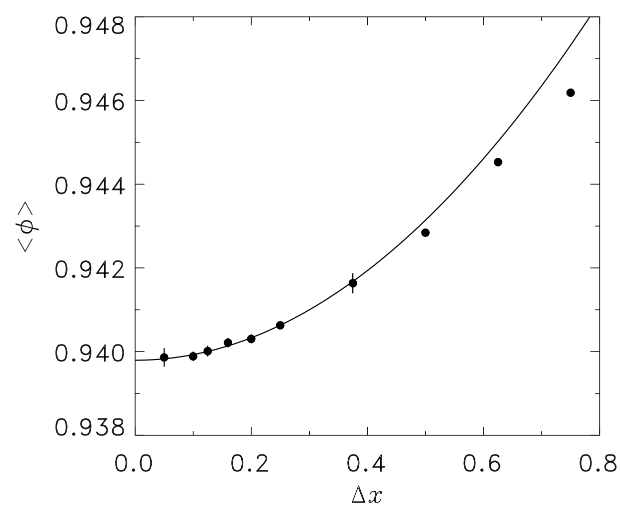

FIG. 5. Space- and time-averaged mean value of ϕ for different values of the lattice spacing Δx. The solid line is the large-β estimate (51) obtained from the Gaussian ansatz (47) with $\beta = 10$, $\eta = 1$. Statistical error bars are not shown if they are smaller than the symbol size.

VI. CONCLUSIONS

We have presented a complete procedure to identify space and time discreteness effects in Langevin studies of 1+1-dimensional field theories on the lattice. This scheme permits the determination of the correct continuum limit of the theory in thermal equilibrium. In particular, we have shown that for the standard spatial discretization of the Langevin equation, quantities of interest such as the kink density and the expectation value of the field and its variance differ from the continuum values by terms of order Δx^2. High resolution numerical results are in excellent agreement with our analytical predictions.

In any numerical Langevin evolution errors result from the necessary discretization of a field theory in both time and space. The effect of the former is to modify the form of the canonical distribution as seen from the solution of the corresponding Fokker-Planck equation. The use of higher order timestepping algorithms can render this error subdominant when compared to errors arising from the discretization of the spatial lattice.

This spatial discretization error can be computed systematically in powers of $(\Delta x)^2$ via the use of the transfer integral to solve for the partition function on the lattice. This procedure leads to the identification of a simple local counterterm which in turn permits the practical elimination of the leading order lattice error in Langevin evolutions at low temperature.

For the ϕ^4 theory in one space dimension, the density of kinks converges to a well-defined value at any temperature low enough that kinks are clearly separated from small wave-length fluctuations (or "phonons"). In practice this is essentially the range of temperatures where the dilute gas approximation (which is equivalent to a WKB solution of the transfer integral) is valid. Precision calculations over a wide range of temperatures that agree with transfer integral predictions are reported in Ref. [11]. For quantities that are defined unambiguously at arbitrary temperatures, such as the correlation length, results based on the WKB approximation to the transfer integral will fail at sufficiently high temperatures. This is independent of lattice errors and does not preclude analytical and numerical study using lattice simulations.

Our results disagree with those reported by Gleiser and Müller based on a one loop counterterm [12]. A critical examination of their proposal has shown that it does not in fact constitute a scheme for the control and elimination of lattice errors. We have also carried out a direct comparison of our numerical results with those presented in Ref. [12] and are led to conclude that their data must have been of insufficient quality to quantitatively characterize lattice spacing dependences.

Finally we wish to note that our methods strongly depend on the use of the transfer integral to solve (exactly) for the non-perturbative field thermodynamics. The application of the procedure described above is in general guaranteed for any (local) field theory in one spatial dimension, requiring only the choice of the appropriate potential.

In higher dimensions such a solution becomes increasingly difficult. Nevertheless, for the particular case of two dimensions several lattice models can be solved exactly, precisely by applying the transfer integral technique [18]. The eigenvalue problem, elegantly posed in terms of an ordinary time-independent Schödinger equation in one dimension, now amounts to solving for the eigenvalues of an infinite matrix. Regardless of this apparent difficulty, exact solutions are known in several interesting cases, most notably perhaps for the 2D Ising model on a square lattice. It is therefore conceivable that the detailed approach to the continuum in these models can be understood via the procedure described above.

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